



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:35 am BST

PDB ID : 3GOL
Title : HCV NS5b polymerase in complex with 1,5 benzodiazepine inhibitor (R)-11d
Authors : Nyanguile, O.; De Bondt, H.
Deposited on : 2009-03-19
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

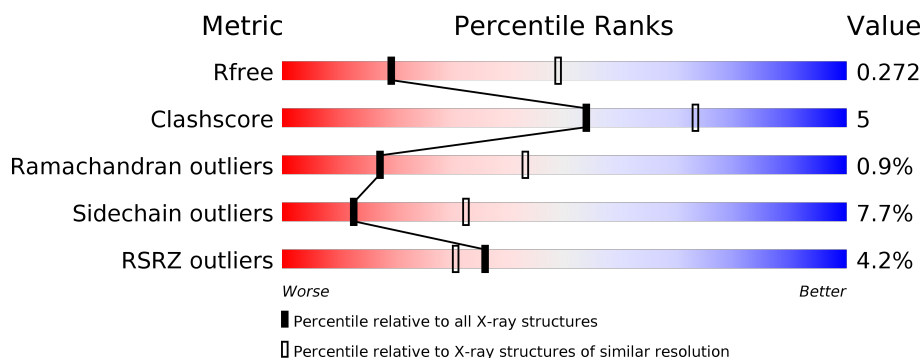
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	581	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 79%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 15% • • </div> </div>
1	B	581	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 1%, yellow 17%, green 78%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 7% 78% 17% • • </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8869 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase.

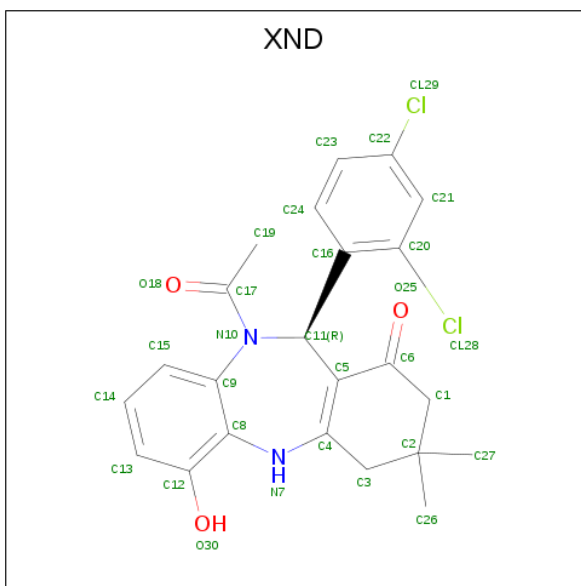
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4337	2732	767	806	32			
1	B	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP O92972
A	-1	ALA	-	EXPRESSION TAG	UNP O92972
A	0	SER	-	EXPRESSION TAG	UNP O92972
A	571	LEU	-	EXPRESSION TAG	UNP O92972
A	572	GLU	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
A	577	HIS	-	EXPRESSION TAG	UNP O92972
A	578	HIS	-	EXPRESSION TAG	UNP O92972
B	-2	MET	-	EXPRESSION TAG	UNP O92972
B	-1	ALA	-	EXPRESSION TAG	UNP O92972
B	0	SER	-	EXPRESSION TAG	UNP O92972
B	571	LEU	-	EXPRESSION TAG	UNP O92972
B	572	GLU	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972
B	577	HIS	-	EXPRESSION TAG	UNP O92972
B	578	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is (11R)-10-acetyl-11-(2,4-dichlorophenyl)-6-hydroxy-3,3-dimethyl-2,3,4,5,10,11-hexahydro-1H-dibenzo[b,e][1,4]diazepin-1-one (three-letter code: XND) (formula:

$C_{23}H_{22}Cl_2N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			30	23	2	2	3		
2	B	1	Total	C	Cl	N	O	0	0
			30	23	2	2	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

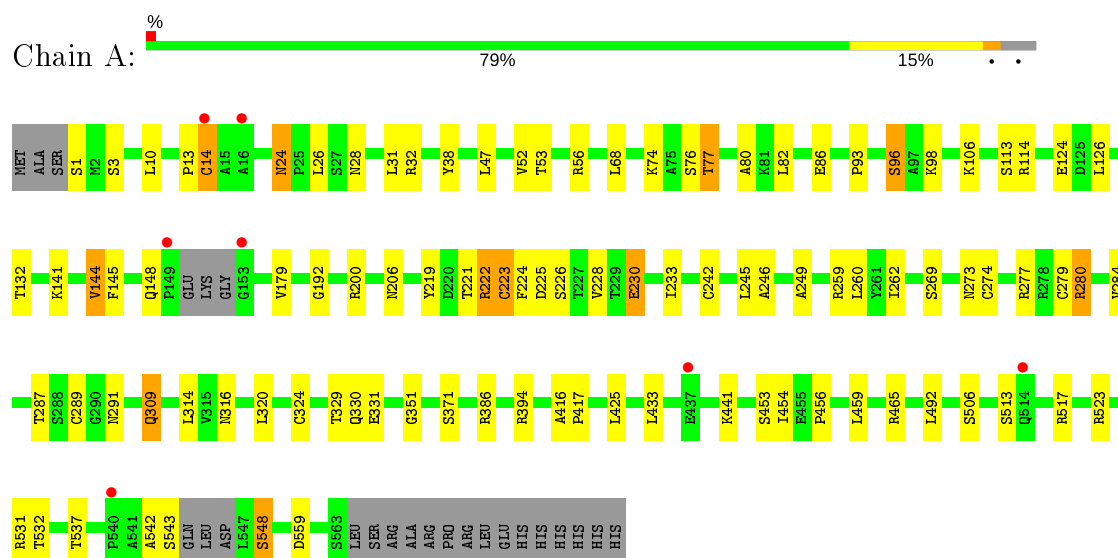
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	40	Total	O	0	0
			40	40		

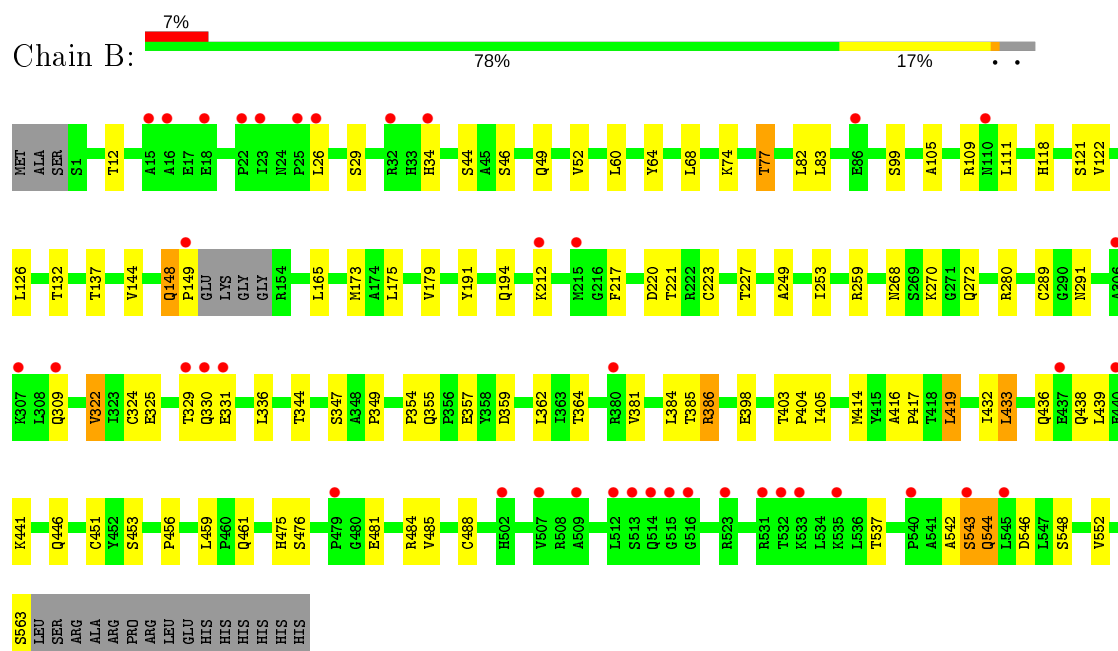
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.05Å 106.62Å 134.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.81 – 2.85 41.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.81-2.85) 99.6 (41.80-2.85)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.250 0.221 , 0.272	Depositor DCC
R_{free} test set	1811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8869	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, XND

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	1/4431 (0.0%)	0.70	2/6012 (0.0%)
1	B	0.54	2/4453 (0.0%)	0.68	0/6044
All	All	0.56	3/8884 (0.0%)	0.69	2/12056 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	CYS	CB-SG	-5.59	1.72	1.81
1	B	451	CYS	CB-SG	-5.47	1.72	1.81
1	B	488	CYS	CB-SG	-5.07	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	280	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	544	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4337	0	4350	41	0
1	B	4358	0	4371	51	0
2	A	30	0	21	1	0
2	B	30	0	21	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	72	0	0	4	0
4	B	40	0	0	5	0
All	All	8869	0	8763	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:SER:HA	1:B:49:GLN:HE21	1.28	0.95
1:B:268:ASN:HD21	1:B:272:GLN:HE21	1.04	0.92
1:B:118:HIS:O	1:B:122:VAL:HG23	1.73	0.88
1:B:268:ASN:HD21	1:B:272:GLN:NE2	1.83	0.76
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.71	0.71
1:B:46:SER:HA	1:B:49:GLN:NE2	2.06	0.70
1:B:132:THR:O	1:B:259:ARG:HD2	1.93	0.69
1:B:476:SER:N	4:B:601:HOH:O	2.25	0.68
1:B:398:GLU:HG2	1:B:403:THR:HG21	1.77	0.67
1:A:82:LEU:HD11	1:A:249:ALA:HB2	1.78	0.65
1:A:284:VAL:O	1:A:287:THR:HG22	1.97	0.65
1:A:132:THR:O	1:A:259:ARG:HD2	1.98	0.63
1:B:212:LYS:N	1:B:325:GLU:OE2	2.34	0.59
1:B:359:ASP:HA	4:B:604:HOH:O	2.03	0.58
1:A:52:VAL:HG22	1:A:226:SER:OG	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HG22	1:A:394:ARG:CG	2.35	0.56
1:B:403:THR:OG1	1:B:404:PRO:HD2	2.06	0.55
1:B:83:LEU:HB2	1:B:173:MET:HA	1.89	0.55
1:A:523:ARG:HD3	4:A:633:HOH:O	2.07	0.55
1:B:433:LEU:HB3	1:B:439:LEU:HD13	1.88	0.55
1:A:82:LEU:CD1	1:A:249:ALA:HB2	2.36	0.55
1:B:309:GLN:O	1:B:324:CYS:HB2	2.07	0.55
1:B:179:VAL:HG13	1:B:289:CYS:HB2	1.90	0.54
1:B:329:THR:HG23	4:B:598:HOH:O	2.08	0.53
1:B:542:ALA:O	1:B:543:SER:C	2.47	0.52
1:B:217:PHE:CZ	1:B:322:VAL:HG11	2.43	0.52
1:B:456:PRO:HA	1:B:459:LEU:HD23	1.92	0.51
1:A:200:ARG:HH21	1:A:316:ASN:ND2	2.08	0.51
1:A:144:VAL:HG22	1:A:394:ARG:HG3	1.93	0.50
1:B:105:ALA:O	1:B:109:ARG:HG3	2.10	0.50
1:B:132:THR:O	1:B:259:ARG:CD	2.57	0.50
1:B:544:GLN:HA	1:B:546:ASP:HB3	1.92	0.50
1:A:456:PRO:HA	1:A:459:LEU:HD13	1.92	0.50
1:A:260:LEU:O	1:A:277:ARG:NH2	2.44	0.49
1:A:28:ASN:ND2	4:A:596:HOH:O	2.44	0.49
1:B:414:MET:HG3	2:B:579:XND:H27B	1.95	0.49
1:B:74:LYS:O	1:B:77:THR:OG1	2.27	0.49
2:A:579:XND:CL28	2:A:579:XND:N10	2.82	0.49
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.95	0.48
1:B:217:PHE:CE1	1:B:322:VAL:HG13	2.48	0.48
1:B:217:PHE:CZ	1:B:322:VAL:CG1	2.96	0.48
1:B:416:ALA:N	1:B:417:PRO:CD	2.77	0.48
1:B:419:LEU:HD23	1:B:485:VAL:HG21	1.94	0.48
1:A:144:VAL:HG22	1:A:394:ARG:HG2	1.95	0.47
1:A:179:VAL:HG22	1:A:289:CYS:CB	2.45	0.47
1:A:223:CYS:O	1:A:224:PHE:C	2.53	0.46
1:B:385:THR:OG1	1:B:386:ARG:N	2.47	0.46
1:B:227:THR:HB	1:B:347:SER:O	2.15	0.45
1:B:268:ASN:ND2	1:B:272:GLN:HE21	1.89	0.45
1:A:280:ARG:HD2	1:A:291:ASN:OD1	2.16	0.45
1:A:74:LYS:O	1:A:77:THR:HB	2.17	0.45
1:A:82:LEU:HD13	1:A:246:ALA:HB3	1.98	0.45
1:B:475:HIS:N	4:B:601:HOH:O	2.46	0.45
1:A:76:SER:HA	1:A:242:CYS:O	2.16	0.45
1:B:148:GLN:HB2	1:B:149:PRO:HD2	1.99	0.44
1:A:200:ARG:HH21	1:A:316:ASN:HD21	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLN:O	1:A:324:CYS:HB2	2.18	0.44
1:B:60:LEU:HD13	1:B:64:TYR:CE2	2.53	0.44
1:A:228:VAL:HG12	1:A:233:ILE:HD11	2.00	0.44
1:A:230:GLU:CD	1:A:262:ILE:HD11	2.38	0.44
1:A:331:GLU:H	1:A:331:GLU:CD	2.21	0.44
1:A:132:THR:O	1:A:259:ARG:CD	2.66	0.43
1:A:386:ARG:NH1	4:A:619:HOH:O	2.51	0.43
1:B:191:TYR:O	1:B:194:GLN:HG2	2.18	0.43
1:B:148:GLN:O	1:B:149:PRO:C	2.57	0.43
1:B:543:SER:OG	1:B:544:GLN:N	2.50	0.43
1:B:99:SER:HB2	1:B:165:LEU:HB3	2.01	0.43
1:B:542:ALA:O	1:B:546:ASP:HB2	2.18	0.43
1:A:38:TYR:CZ	1:A:145:PHE:HB2	2.54	0.43
1:A:543:SER:C	4:A:632:HOH:O	2.56	0.43
1:B:12:THR:HG21	1:B:270:LYS:HZ2	1.84	0.42
1:A:93:PRO:HD3	1:A:559:ASP:O	2.19	0.42
1:A:96:SER:OG	1:A:559:ASP:OD1	2.36	0.42
1:B:26:LEU:HD22	1:B:432:ILE:HD12	2.01	0.42
1:B:82:LEU:HD13	1:B:249:ALA:HB2	2.01	0.42
1:B:344:THR:HG23	1:B:349:PRO:HB3	2.02	0.42
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.41
1:A:192:GLY:HA2	1:A:314:LEU:HD11	2.02	0.41
1:A:3:SER:OG	1:A:53:THR:HA	2.20	0.41
1:B:336:LEU:HD21	1:B:354:PRO:HG2	2.01	0.41
1:A:531:ARG:CG	1:A:532:THR:N	2.83	0.41
1:B:481:GLU:HB2	4:B:613:HOH:O	2.20	0.41
1:B:26:LEU:HD22	1:B:432:ILE:CD1	2.50	0.41
1:A:225:ASP:O	1:A:279:CYS:HB2	2.20	0.41
1:A:80:ALA:HB3	1:A:245:LEU:HD23	2.03	0.41
1:B:359:ASP:HB3	1:B:362:LEU:HD22	2.03	0.41
1:B:436:GLN:HE21	1:B:438:GLN:HG3	1.85	0.41
1:B:46:SER:CA	1:B:49:GLN:HE21	2.15	0.41
1:A:453:SER:C	1:A:454:ILE:HG13	2.41	0.40
1:B:280:ARG:HD2	1:B:291:ASN:OD1	2.21	0.40
1:A:24:ASN:ND2	1:A:26:LEU:H	2.18	0.40
1:A:230:GLU:HB2	1:A:262:ILE:HG12	2.03	0.40
1:A:31:LEU:HD11	1:A:492:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/581 (95%)	517 (94%)	28 (5%)	6 (1%)	14	38
1	B	555/581 (96%)	517 (93%)	34 (6%)	4 (1%)	22	50
All	All	1106/1162 (95%)	1034 (94%)	62 (6%)	10 (1%)	17	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ARG
1	A	548	SER
1	B	543	SER
1	A	14	CYS
1	A	13	PRO
1	A	542	ALA
1	B	419	LEU
1	B	441	LYS
1	A	351	GLY
1	B	552	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/495 (96%)	434 (92%)	40 (8%)	11	28
1	B	477/495 (96%)	444 (93%)	33 (7%)	15	38
All	All	951/990 (96%)	878 (92%)	73 (8%)	13	32

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	10	LEU
1	A	14	CYS
1	A	24	ASN
1	A	32	ARG
1	A	47	LEU
1	A	56	ARG
1	A	68	LEU
1	A	77	THR
1	A	86	GLU
1	A	96	SER
1	A	98	LYS
1	A	106	LYS
1	A	113	SER
1	A	114	ARG
1	A	124	GLU
1	A	126	LEU
1	A	141	LYS
1	A	144	VAL
1	A	148	GLN
1	A	206	ASN
1	A	221	THR
1	A	222	ARG
1	A	230	GLU
1	A	269	SER
1	A	273	ASN
1	A	274	CYS
1	A	309	GLN
1	A	329	THR
1	A	330	GLN
1	A	371	SER
1	A	425	LEU
1	A	433	LEU
1	A	441	LYS
1	A	465	ARG
1	A	506	SER
1	A	513	SER
1	A	517	ARG
1	A	537	THR
1	A	548	SER
1	B	29	SER
1	B	34	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	44	SER
1	B	52	VAL
1	B	68	LEU
1	B	77	THR
1	B	111	LEU
1	B	121	SER
1	B	126	LEU
1	B	137	THR
1	B	144	VAL
1	B	148	GLN
1	B	220	ASP
1	B	221	THR
1	B	223	CYS
1	B	322	VAL
1	B	330	GLN
1	B	331	GLU
1	B	355	GLN
1	B	357	GLU
1	B	364	THR
1	B	381	VAL
1	B	384	LEU
1	B	386	ARG
1	B	405	ILE
1	B	433	LEU
1	B	446	GLN
1	B	453	SER
1	B	461	GLN
1	B	484	ARG
1	B	537	THR
1	B	548	SER
1	B	563	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	28	ASN
1	A	34	HIS
1	A	35	ASN
1	A	148	GLN
1	A	273	ASN
1	A	316	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	355	GLN
1	A	483	ASN
1	B	49	GLN
1	B	206	ASN
1	B	272	GLN
1	B	316	ASN
1	B	436	GLN
1	B	446	GLN
1	B	461	GLN
1	B	483	ASN
1	B	562	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XND	A	579	-	32,33,33	1.16	4 (12%)	48,51,51	1.66	7 (14%)
2	XND	B	579	-	32,33,33	1.11	3 (9%)	48,51,51	1.43	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XND	A	579	-	-	1/8/42/42	0/3/4/4
2	XND	B	579	-	-	0/8/42/42	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	XND	C17-N10	3.16	1.43	1.37
2	A	579	XND	C3-C4	3.11	1.53	1.50
2	B	579	XND	C3-C4	2.84	1.53	1.50
2	B	579	XND	C16-C11	2.70	1.55	1.52
2	A	579	XND	C11-C5	2.56	1.54	1.51
2	A	579	XND	C16-C11	2.43	1.55	1.52
2	B	579	XND	C6-C5	2.33	1.50	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	XND	C8-C9-N10	5.50	122.68	119.26
2	A	579	XND	C19-C17-N10	3.61	123.06	117.86
2	A	579	XND	C9-N10-C11	-3.46	113.41	118.94
2	B	579	XND	C2-C1-C6	-3.41	109.42	114.48
2	B	579	XND	C8-C9-N10	3.25	121.28	119.26
2	A	579	XND	C5-C4-N7	-3.18	124.86	126.71
2	A	579	XND	C2-C1-C6	-3.17	109.78	114.48
2	B	579	XND	C19-C17-N10	3.01	122.19	117.86
2	A	579	XND	C12-C8-N7	-2.99	114.26	118.92
2	B	579	XND	C3-C4-C5	-2.79	120.01	123.43
2	B	579	XND	C9-N10-C11	-2.43	115.05	118.94
2	B	579	XND	C2-C3-C4	2.36	116.05	113.40
2	B	579	XND	C3-C4-N7	2.04	113.60	111.98
2	A	579	XND	C24-C16-C20	2.00	118.80	116.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

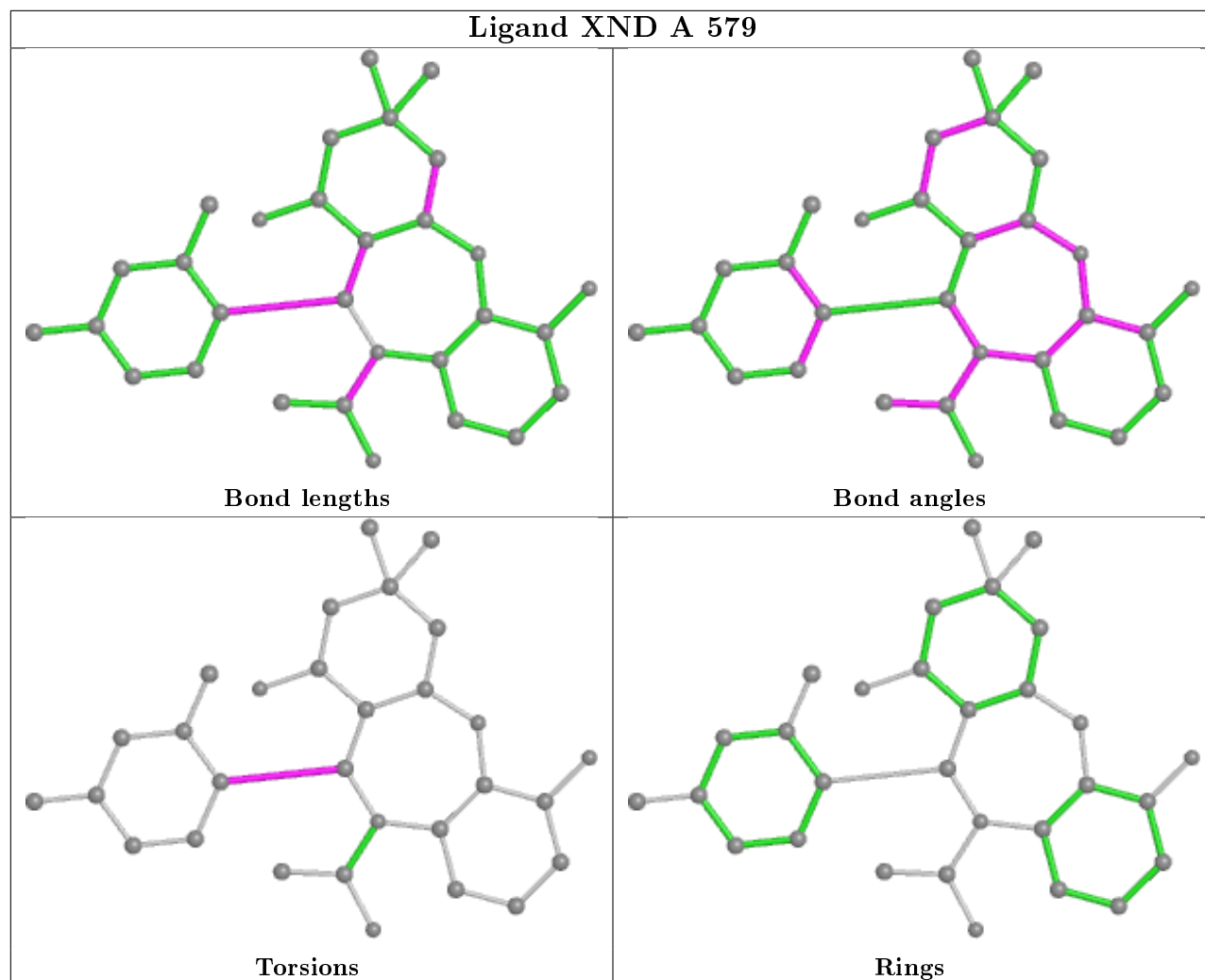
Mol	Chain	Res	Type	Atoms
2	A	579	XND	N10-C11-C16-C20

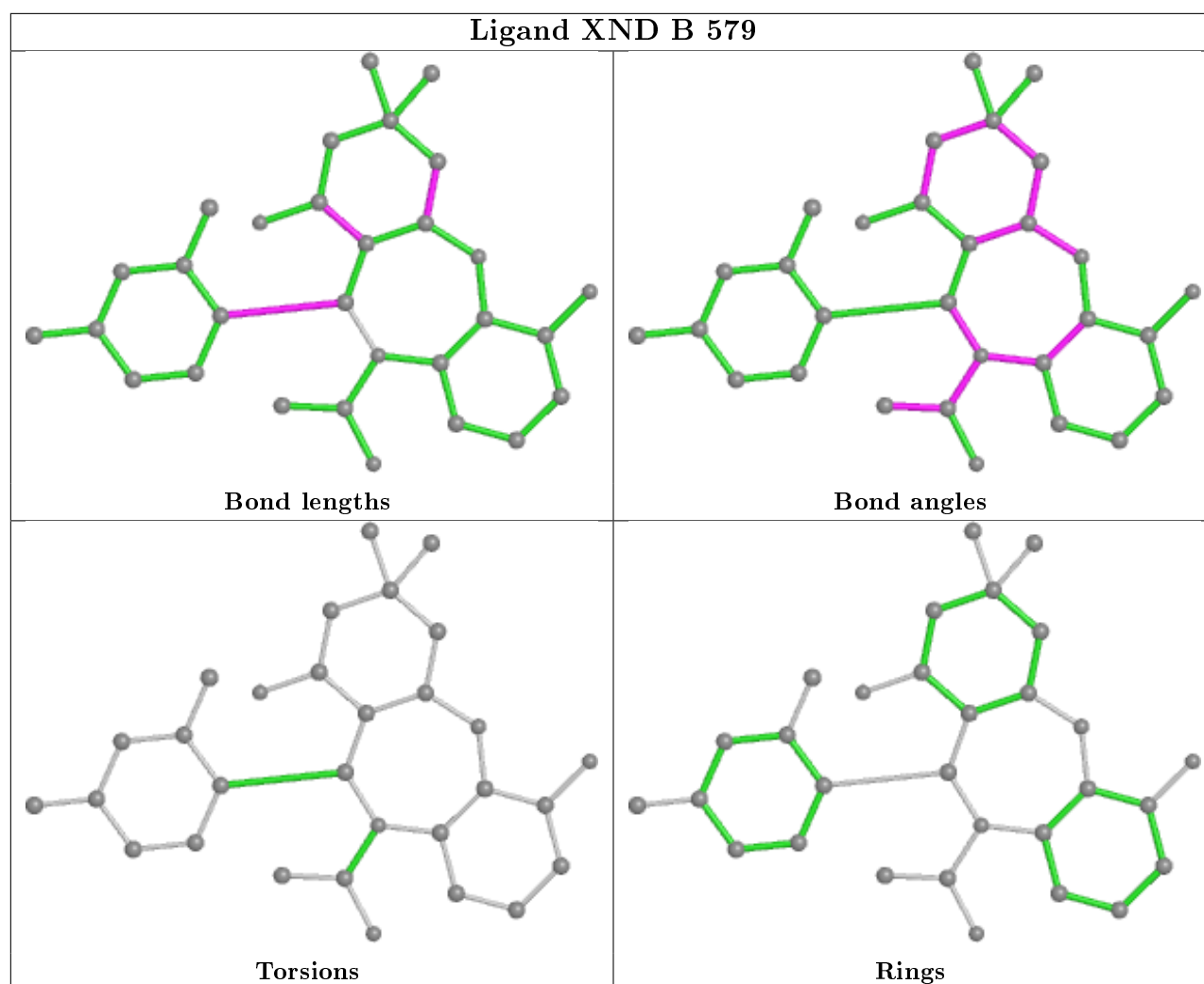
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	XND	1	0
2	B	579	XND	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/581 (95%)	0.09	7 (1%) 77 76	21, 34, 49, 66	0
1	B	559/581 (96%)	0.31	40 (7%) 15 11	20, 34, 49, 59	0
All	All	1116/1162 (96%)	0.20	47 (4%) 36 31	20, 34, 49, 66	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	532	THR	4.6
1	B	23	ILE	4.0
1	B	543	SER	3.8
1	B	513	SER	3.7
1	B	515	GLY	3.5
1	B	440	GLU	3.4
1	B	535	LYS	3.4
1	A	149	PRO	3.4
1	B	531	ARG	3.4
1	B	26	LEU	3.2
1	B	329	THR	3.1
1	A	14	CYS	2.8
1	B	330	GLN	2.7
1	B	514	GLN	2.7
1	B	516	GLY	2.7
1	A	437	GLU	2.7
1	B	212	LYS	2.7
1	B	15	ALA	2.6
1	B	25	PRO	2.6
1	A	16	ALA	2.6
1	B	307	LYS	2.6
1	B	16	ALA	2.6
1	B	540	PRO	2.5
1	B	32	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	540	PRO	2.4
1	B	86	GLU	2.4
1	B	502	HIS	2.4
1	B	331	GLU	2.4
1	B	507	VAL	2.4
1	B	512	LEU	2.3
1	A	153	GLY	2.3
1	B	149	PRO	2.3
1	A	514	GLN	2.3
1	B	34	HIS	2.3
1	B	380	ARG	2.2
1	B	509	ALA	2.2
1	B	523	ARG	2.2
1	B	22	PRO	2.2
1	B	437	GLU	2.2
1	B	306	ALA	2.2
1	B	309	GLN	2.1
1	B	110	ASN	2.1
1	B	545	LEU	2.1
1	B	18	GLU	2.1
1	B	479	PRO	2.1
1	B	533	LYS	2.1
1	B	215	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Continued on next page...

Continued from previous page...

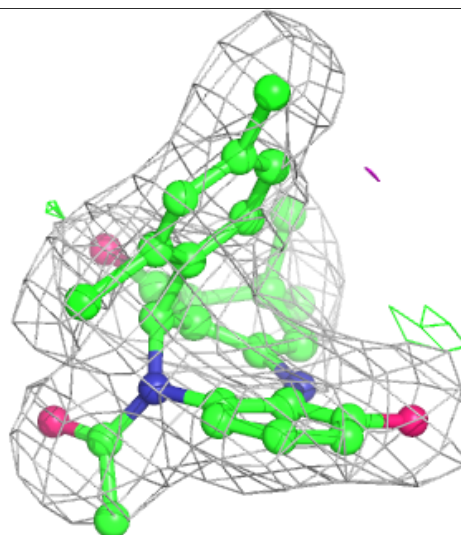
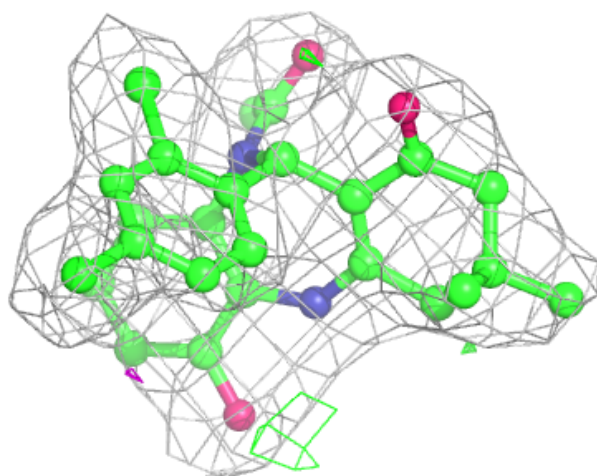
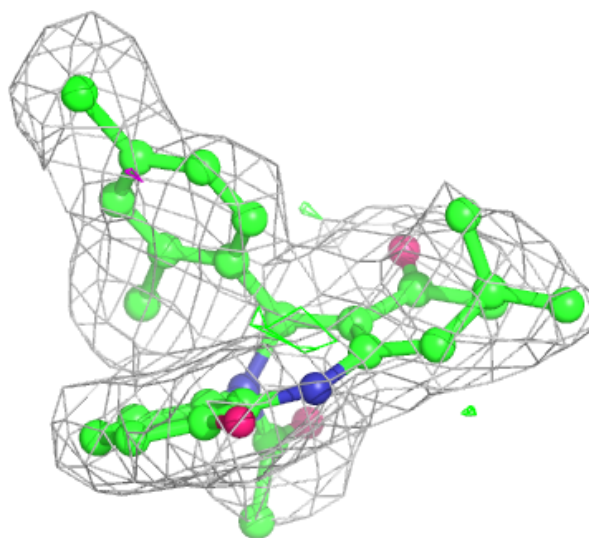
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	580	1/1	0.83	0.16	55,55,55,55	0
3	MG	B	580	1/1	0.85	0.13	40,40,40,40	0
2	XND	A	579	30/30	0.96	0.18	17,24,38,47	0
2	XND	B	579	30/30	0.96	0.17	25,40,52,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

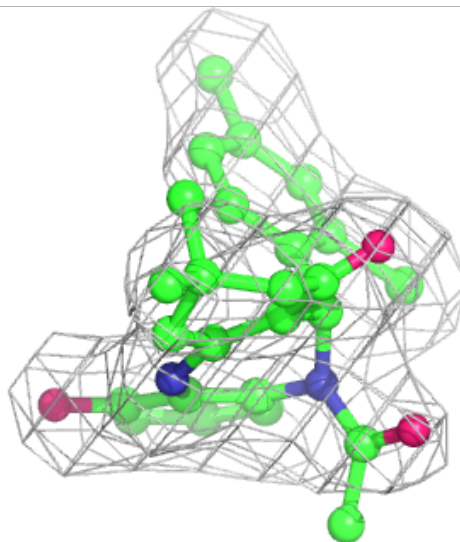
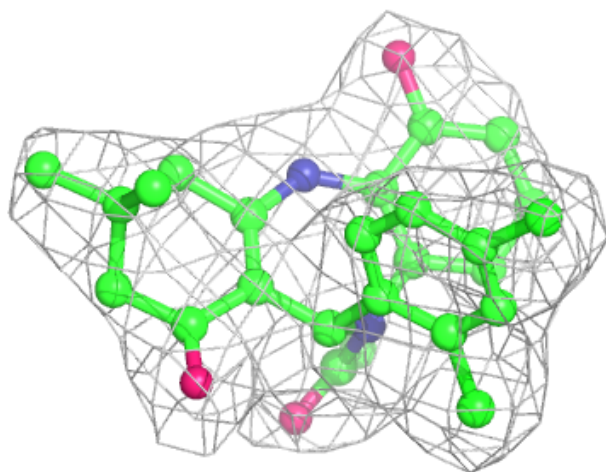
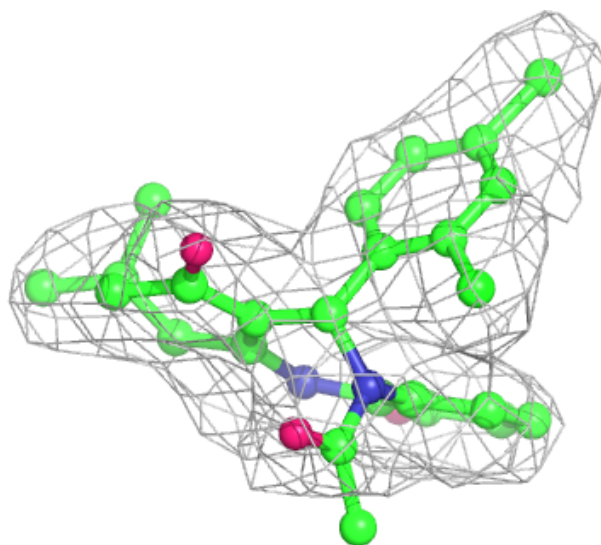
Electron density around XND A 579:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XND B 579:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.